Time-evolution stability of order parameters and phase diagrams of bosons on optical lattice

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Stemming from the Heisenberg equations of motion, we study the time-evolution stability of the order parameters for the cold atoms on optical lattices. The requirement of this stability of the order parameters endows the phase diagram with a fruitful structure in the superfluid phase. For the one-component Bose-Hubbard model, we see that this stability of order parameter leads to a physically receivable phase diagram. For two-component bosons, we show that the molecules are preformed in the atomic superfluid and then condenses into a molecular superfluid phase at a critical repulsive inter-species interaction, which resembles the pre-pairing mechanism in high T_c superconductor of Cu-O cuprates.

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Ultra-cold atoms on optical lattices have offered a paradigmatic scene to study strongly correlated phenomenon in a highly controllable environment[1, 2, 3, 4]. Superfluid/Mott-insulator transition was witnessed on ^{87}Rb atoms in a three- [2] and one-dimensional lattice [4]. Theoretically, the strongly correlated phenomenon for boson systems may be studied by the Bose-Hubbard model [5], and experimental feasibility was also established by microscopic calculations of the model parameters for cold boson atoms in optical lattices [6].

Very fruitful structures of the phase diagram have been explored . The phase boundary between the superfluid and the Mott insulator has been determined [7] and verified by the experiments [2, 4]. In the Mott insulator, the Bose-Hubbard model can be mapped into an effective spin Hamiltonian and the phase structure has been extensively studied [9]. On the superfluid side, it is also predicted that there are complex quantum phase transitions [9, 10].

The Bose-Hubbard model can only be exactly solved in one-dimension for a limited case. Various approximations have been applied. If an approximation ground state describes a spontaneous breaking of symmetry, it has to be stable in the time-evolution. A powerful tool to study this stability is the Heisenberg equations of motion of the corresponding order parameter operator. For any equilibrium state described by a time-independent density matrix ρ with $[H,\rho]=0$, the Heisenberg equation of motion of an operator O yields

$$-i\langle\dot{O}\rangle=\langle[H,O]\rangle=\mathrm{Tr}(\rho[H,O])=0, \qquad (1)$$

which gives the exact constraint on order parameter: When an approximation state is readily to describe an ordered state, one has to check that the corresponding order parameter is stable or not in the sense obeying (1). The first such example has been provided by Zhang for the Hubbard model of the electrons and it has been generalized to the t-J model [11]. These works suggested that the Hubbard model may not be a good model for the high T_c superconductor while the t-J model is possible.

For bosons on the lattice, we shall show that similar exact constraints on the order parameters play an important role in the study of the phase structures of the systems. We shall use the variational wave function which yields the mean field state for Bose-Hubbard systems [10, 12]. It is seen that the variational energy will be affected by the constraint on the corresponding order parameter. We shall see that even for the simplest one-component Bose-Hubbard model, these exact results lead to a more physically receivable phase diagram. For the two-component Bose-Hubbard model with a commensurate filling, the most intriguing finding is that except the up-critical point from the superfluid to the Mott insulator, there is a phase transition from the atomic superfluid (AS) to the molecular superfluid(MS) in a low-critical point for a repulsive inter-species interaction. The existence of the MS phase for $U>0$ is because the local $n_i=1$ is violated in the superfluid and $V>U$ favors two atoms in different species to form a molecule. Our analysis will show that the molecules are formed in the AS phase and condensed as U reduces to a critical value, which resembles the prepairing mechanism for the high T_c superconductivity. To be specific, we confine our discussions to the single atom filling per lattice site in this work. However, it is easy to be generalized to other integer filling factors and the mixture of the Bose-Fermi atoms.

One-component model: We now begin with the one-component Bose-Hubbard model, which is described by the Hamiltonian

$$H_1=-t\sum_{\langle ij\rangle}(a_i^\dagger a_j+\mathrm{h.c.})+\frac{V}{2}\sum_i n_i(n_i-1)-\mu\sum_i n_i, \qquad (2)$$

where the notation is standard. For the uniform order parameters, the Heisenberg equations of motion for a and a^2 give

$$\begin{aligned}-i\langle\dot{a}\rangle &= tz\langle a\rangle-V\langle na\rangle+\mu\langle a\rangle,\\ -i\langle\dot{a^2}\rangle &= 2tz\langle a_\delta a\rangle+2\mu\langle a^2\rangle-V\langle na^2\rangle, \qquad (3)\end{aligned}$$

where a_δ is the boson operator at a nearest neighbor and z is the partition number. Precisely, the superfluid and dimerized order parameters are defined by $\langle a\rangle = \mathrm{Tr}(\rho a)$ and $\langle a^2\rangle = \mathrm{Tr}(\rho a^2)$. In the zero temperature limit, they are reduced to the expectation value corresponding to the ground state. In the dilute gas limit, a widely accepted approxiamtion is, instead of the exact ground state, to introduce a site factorizable wave function which takes the form [12]

$$|\Phi_1\rangle = \prod_i \left[\sin\frac{\theta_i}{2}a_i^\dagger + \cos\frac{\theta_i}{2}\left(\sin\frac{\chi_i}{2} + \frac{1}{\sqrt{2}}\cos\frac{\chi_i}{2}a_i^{\dagger 2}\right)\right]|0\rangle. \quad (4)$$

We confine the filling number per site to be one throughout this work. The order parameters now are $\langle a\rangle = (2+\sqrt{2})\sin\theta/(2\sqrt{2})$ and $\langle a^2\rangle = \cos^2\frac{\theta}{2}/\sqrt{2}$ since $\chi = \pi/2$ when the order parameters do not vanish and $\langle n\rangle = 1$. If we do not consider the time evolution of the order parameters, there are three possible phase: the Mott insulator phase with $\theta = \pi$ ($\langle a\rangle = \langle a^2\rangle = 0$), the dimerized phase with $\theta = 0$ ($\langle a\rangle = 0$ and $\langle a^2\rangle \neq 0$) and the superfluid phase with both $\langle a\rangle \neq 0$ and $\langle a^2\rangle \neq 0$. If taking the chemical potential μ as a constant, the previous variational result has shown the critical points of the SF/MI and SF/D are in $V/zt \approx \pm 5.83$ [7]. The plus one is reasonable and has been examined experimentally. The minus one seems to be a mean field artifact because it was known that in the one-dimensional model, the dimerized state dominates when $V/zt \leq -1$ for $V < 0$ [8]. To improve the result from this simple mean field theory, we consider the stability of the order parameters in time evolution. There are now two different variational states in superfluid phase. One is that $\langle a\rangle$ is stable and $\langle a^2\rangle$ is not and another is vice verse. The former subjects to the constraint $-i\langle\dot{a}\rangle = 0$ which turns the first equation of (3) to $\mu = \mu_1 = -tz + V(\sqrt{2}-1)$. The latter to $-i\langle a^2\rangle = 0$, which turns to $\mu = \mu_2 = -\frac{3+2\sqrt{2}}{\sqrt{2}}tz\sin^2\frac{\theta}{2}$. The variational energies to be minimized are

$$E_{s1,s2}(\theta) = -\frac{3+2\sqrt{2}}{8}tz\sin^2\theta + \frac{V}{2}\cos^2\frac{\theta}{2} - \mu_{1,2}. \quad (5)$$

Minimizing these variational energies, the optimizing parameter is given by

$$\cos\theta_1 = -\frac{V}{tz(3+2\sqrt{2})}, \quad \cos\theta_2 = \sqrt{2} - \frac{V}{tz(3+2\sqrt{2})}. \quad (6)$$

The requirement $|\cos\theta_{1,2}| \leq 1$ gives the regimes of the minimal $E_{1s,2s}$ defined: $V_{1,2}^{(-)} \leq V \leq V_{1,2}^{(+)}$ with $V_1^{(\pm)}/zt \approx \pm 5.83$ and $V_2^{(\pm)}/zt \approx 5.83(\sqrt{2}\pm 1)$. Outside of these ranges, the energies are defined by $E_{1,2}(\theta = 0, \pi)$. Thus, corresponding to two cases, the optimizing energies are

$$\begin{aligned} E_{1,2} &= E_{s1,s2}(\theta=0)\Theta(V_{1,2}^{(-)} - V) \\ &+ E_{s1,s2}(V/tz)\Theta(V - V_{1,2}^{(-)})\Theta(V_{1,2}^{(+)} - V) \\ &+ E_{s1,s2}(\theta=\pi)\Theta(V - V_{1,2}^{(+)}), \end{aligned} \quad (7)$$

where $\Theta(x)$ is the step function. We depict these energies in Fig. 1(a). It is found that in the whole range where $\langle a\rangle \neq 0$, $E_2 > E_1$. However, at the point $V/zt \approx -0.4$, $E_2 = E_1$. This gives that the lower critical point of SF/D transition. The whole phase diagram of the system is shown in Fig. 1(b). There are three phases which are identical to those in Fig. 1 (b). The phase with stable $\langle a^2\rangle \neq 0$ and nonzero but unstable $\langle a\rangle$ does not exist. However, due to the energy of the dimerized phase is lowered, the phase boundary between SF-D and D is shifted a much reasonable value $V/tz \approx -0.4$.

In our variational state, the states with three or more atoms per site have been neglected. For a repulsive interaction, this approximation is appropriate because there was a large three-body collision loss in experiment. For a large negative V or denser atoms, the order parameters $\langle a^n\rangle$ ($n \geq 3$) are possibly stable. We can use the procedure provided before to discuss. Our procedure can also be applied to the other integer filling by taking an appreciate variational wave function.

Two-component model: Turn to the two-component Bose-Hubbard model. The Hamiltonian is given by

$$\begin{aligned} H_2 &= -\sum_{\langle ij\rangle;\sigma=\uparrow,\downarrow} t_\sigma(a_{i\sigma}^\dagger a_{j\sigma} + \text{h.c.}) + \frac{1}{2}\sum_{i,\sigma} V_\sigma n_{i\sigma}(n_{i\sigma}-1) \\ &+ U\sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) - \sum_{i\sigma}\mu_\sigma n_{i\sigma}. \end{aligned} \quad (8)$$

Generally, the tunneling amplitudes $t_{\uparrow,\downarrow}$, the intra-species interactions $V_{\uparrow,\downarrow}$ may be different. It was known that if $V_\uparrow V_\downarrow < U^2$, one can not minimize the ground state energy with two nonzero occupation numbers $\langle n_{\uparrow,\downarrow}\rangle$. The system must be phase separated [13]. We shall not discuss the phase separation here and consider only the interactions restricted in $V_\sigma > 0$ and $V_\uparrow V_\downarrow > U^2$ if $U > 0$. For $U < 0$, the phase diagram has been extensively studied and we shall not go to the details here [9, 14]. The total atom number is conserved in the system and the ratio between the different species atom numbers is self-consistently determined by the internal field and the constraints given rise to by the Heisenberg equations of motion. We now have five possible order parameters, $\langle a_\sigma\rangle$, $\langle a_\uparrow a_\downarrow\rangle$ and $\langle a_\sigma^2\rangle$ if we fix the filling factor per site to one and neglect the three or more atom occupation in a single site. The time-evolutions of the order parameters are given by

$$\begin{aligned} -i\langle\dot{a}_\sigma\rangle &= (zt_\sigma + \mu_\sigma + \frac{U}{2})\langle a_\sigma\rangle - U\langle n_{\bar\sigma}a_\sigma\rangle - V_\sigma\langle n_\sigma a_\sigma\rangle, \\ -i\langle\dot{a^2}_\sigma\rangle &= (2zt_\sigma + 2\mu_\sigma + U)\langle a_{\delta,\sigma}a_\sigma\rangle - 2U\langle n_{\bar\sigma}a_\sigma^2\rangle \\ &\quad - V_\sigma\langle n_\sigma a_\sigma^2\rangle, \\ -i\langle\dot{(a_\uparrow a_\downarrow)}\rangle &= \frac{1}{2}z(t_\uparrow + t_\downarrow)(\langle a_{\delta,\uparrow}a_\downarrow\rangle + \langle a_{\delta,\downarrow}a_\uparrow\rangle) \\ &\quad + (\frac{V}{2} - U)\langle n a_\uparrow a_\downarrow\rangle + (\mu_\uparrow + \mu_\downarrow)\langle a_\uparrow a_\downarrow\rangle. \end{aligned} \quad (9)$$

The most general factorable variational wave function in

our case is that

$$|\Phi_2\rangle = \prod_i \Big[\sin\frac{\theta_i}{2}\Big(\sin\frac{\chi_i}{2}a_{i\uparrow}^\dagger + \cos\frac{\chi_i}{2}a_{i\downarrow}^\dagger\Big) + \cos\frac{\theta_i}{2}\Big(\sin\frac{\eta_i}{2} + \cos\frac{\eta_i}{2}\Big(\sin\frac{\xi_i}{2}a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger + \frac{1}{\sqrt{2}}\Big(\sin\frac{\zeta_i}{2}a_{i\uparrow}^{\dagger 2} + \cos\frac{\zeta_i}{2}a_{i\downarrow}^{\dagger 2}\Big)\Big)\Big)\Big]|0\rangle. \quad (10)$$

Note that this factorable assumption implies that an approximation neglecting all the spatial correlations. Thus, the BCS-type state may not appear in our phase diagram although it is a possible ground state [14]. The condition $\langle n\rangle = 1$ fixes $\eta = \pi/2$ if $\theta \neq \pi$. The Mott insulator phase for this Hamiltonian and the variational wave function have been extensively studied by authors of Ref. [9]. We here focus on the homogenous state although we can not exclude the inhomogenous states such as spin glass and so no. They are the atomic superfluid state with $\langle a_\sigma\rangle \neq 0$, the molecular superfluid state with $\langle a_\uparrow a_\downarrow\rangle \neq 0$ and the dimerized state with $\langle a_\sigma^2\rangle \neq 0$.

In terms of (9), the constraint identities may be obtained by requiring the stability of these order parameters. The variational energy now is given by

$$E = -t_\uparrow z\langle a_\uparrow\rangle^2 - t_\downarrow z\langle a_\downarrow\rangle^2 + U\langle n_\uparrow n_\downarrow\rangle - \frac{U}{4} + \frac{\langle n_\uparrow^2\rangle + \langle n_\downarrow^2\rangle}{2} - (V_\uparrow/2 + \mu_\uparrow)\langle n_\uparrow\rangle + (V_\downarrow/2 + \mu_\downarrow)\langle n_\downarrow\rangle, \quad (11)$$

where μ_σ are restricted by the stability requirement of the order parameters. All expectation values in (9) and (11) may be straightforwardly calculated according to the variational wave function (10).

The phase diagram may obtained by solving the constraint equations for the stable order parameter and minimizing the variational energy (11). To save the space, we do not discuss strongly asymmetric case with $t_\uparrow/V_\uparrow \ll t_\downarrow/V_\downarrow$ in which one-component bosons may in the Mott phase while the other is in the superfluid phase. We focus on the species-symmetric model with $t_\uparrow = t_\downarrow = t$ and $V_\uparrow = V_\downarrow = V$. The symmetry requires that the order parameters are species-independent and leads to $\mu_\uparrow = \mu_\downarrow = \mu$ and $\chi = \zeta = \pi/2$. The variational parameters are reduced to θ and ξ only. Corresponding to the stability of non-zero $\langle a_\uparrow\rangle = \langle a_\downarrow\rangle$, $\langle a_\uparrow^2\rangle = \langle a_\downarrow^2\rangle$, or $\langle a_\uparrow a_\downarrow\rangle$, the constraint identities are

$$\begin{aligned}
&(zt + \mu + U/2)\Big(1 + \sin\frac{\xi}{2} + \cos\frac{\xi}{2}\Big) = U\Big(\sin\frac{\xi}{2} + \cos\frac{\xi}{2}\Big),\\
&zt\sin^2\frac{\theta}{2}\Big(1 + \sin\frac{\xi}{2} + \cos\frac{\xi}{2}\Big)^2 + 2(\mu + U/2)\cos\frac{\xi}{2} = 0,\\
&zt\sin^2\frac{\theta}{2}\Big(1 + \sin\frac{\xi}{2} + \cos\frac{\xi}{2}\Big)^2 + 2\mu\sin\frac{\xi}{2} = 0. \quad (12)
\end{aligned}$$

And the variational energy reads

$$E = -\frac{tz}{8}\sin^2\theta\Big(1 + \sin\frac{\xi}{2} + \cos\frac{\xi}{2}\Big)^2 + \frac{1}{2}\cos^2\frac{\theta}{2}\Big(V\cos^2\frac{\xi}{2} + U\sin^2\frac{\xi}{2}\Big) - \mu - \frac{U-V}{4}. \quad (13)$$

Two cases are analytically solvable. One is the hard-core limit in which $V/U \to \infty$ and another is the critical point of the phase separation, $U = V$. In the hard-core limit, the energies are minimized at $\xi = \pi$. This gives $\langle a_\sigma^2\rangle = 0$ as it should be in the hard-core limit. The atomic superfluid phase (AS/MS) corresponding to the first constraint in (12) is confined $-1 < U/4tz < 1$ while the molecular superfluid phase (MS/AS) to the last constraint in (12) is confined $0 < U/4tz < 2$. The variational energies corresponding to these two order parameters in the whole regime of the interaction U may be given by in a similar form as (7). Comparing these two energies for any given $U/4zt$, the phase diagram in the hard-core limit for the symmetric model can be determined (see Fig. 2(a)). The four phases can detected: the molecular superfluid phase and the mixture of the stable molecular superfluid and unstable atomic superfluid phases, these two phases corresponds to the s-wave superconductivity. The mixture of the stable atomic superfluid and unstable molecular superfluid phases, which corresponds to the preparing (but d-wave) for the electrons in high T_c materials ; and the Mott insulator phase. The boundary of the second and third ones is in $U/4zt = 0.5$.

For any finite U/V, to keep the variational energy having a lower bound, the second and third constraints in (12) can only be satisfied if $\theta = 0$, and $\mu = -U/2$ and 0, respectively. In the critical point of phase separation, $U = V$, $E_2 = 3V/2$ for the second constraint and $E_3 = V$ for the third one and then the dimerized phase is always unfavorable. The energy corresponding to the first constraint is minimized at $\xi = \pi/2$. We compare E_3 and E_1 which are in a similar form as (7) and the phase diagram can be depicted (see Fig. 2(b)).

For a general finite $U/V < 1$, the variational energies may be numerically minimized and the phase diagrams are plotted in Fig. 2(b) for $U > 0$. It is seen that the 'MS/AS-D' phase can only exist in the hard-core limit. For a finite V/U, this phase is suppressed and turns to the 'MS' phase. However, as V reduces, the atomic superfluid phase 'AS/MS-D' grows in both directions. In our variational state, the suppression of the Mott phase is not so strong when $V/U \leq 1.73$.

We now discuss the asymmetric case in the hard-core limit. For $t_\uparrow \neq t_\downarrow$, we find that the atomic superfluid state with a stable $\langle a_\sigma\rangle$ exists for $-\frac{1}{2} - \frac{1}{2\sin\chi_0} + \frac{\Delta t\tan\chi_0}{2} < \frac{U}{2z(t_\uparrow + t_\downarrow)} < \frac{1}{2} + \frac{1}{2\sin\chi_0} + \frac{\Delta t\tan\chi_0}{2}$, with χ_0 is the solution of the equation $\frac{1}{4(1+\sin\chi)} + \frac{U\sin\chi}{2z(t_\uparrow+t_\downarrow)(1+\sin\chi)} + \frac{\Delta t\cos\chi}{2(1+\sin\chi)} + \frac{2U}{z(t_\uparrow+t_\downarrow)} = \Delta t\tan\chi$ and $\Delta t = \frac{t_\uparrow - t_\downarrow}{t_\uparrow + t_\downarrow}$. Solving the equation of χ, one finds that there is only a minor modification to that uses the simple variational method taking

$\mu_\sigma = 0$. The latter gives $|U|/2z(t_\uparrow + t_\downarrow) < 1$ [9] and the former, even for $\Delta t = \pm 1$, $|U|/2z(t_\uparrow + t_\downarrow) < 0.97$. At the other critical points, one also finds the critical values of $|U|/2z(t_\uparrow + t_\downarrow)$ does not leave far from their symmetric ones. Thus, we can think the basic feature of the phase structure of superfluid phase in the hard-core limit can mostly be described by the symmetric model. For finite V_σ, the situation may be more complicated, e.g., for the strongly asymmetric case, there is a mixture between the Mott insulator in the one species and the superfluid in the other (see, [9], Chen and Wu at [13]). We shall leave this for coming works.

Finally, we comment on the counterflow superfluid (see Kuklov et al in [9]). The corresponding order parameter is $\langle a_\uparrow^\dagger a_\downarrow \rangle = \frac{1}{2}[\sin^2\frac{\theta}{2}\sin\chi + \sqrt{2}\cos^2\frac{\theta}{2}\sin\xi\cos^2\frac{\eta}{2}(\sin\frac{\zeta}{2} + \cos\frac{\zeta}{2})]$. For $\theta = \pi$, the Mott state, $\langle a_\uparrow^\dagger a_\downarrow \rangle = (1/2)\sin\chi$. However, this mean field order parameter is not stable because the Heisenberg equation of motion $-i\dot{\langle}(a_\uparrow^\dagger a_\downarrow)\rangle = V(\langle(n_\uparrow - n_\downarrow)a_\uparrow^\dagger a_\downarrow\rangle) = V\langle a_\uparrow^\dagger a_\downarrow\rangle$ for the Mott state. In the symmetric model, it holds for arbitrary U and $V0$. Thus, from a mean field point of view, the counterflow superfluid is stable only in a time scale $t \ll 1/V$.

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Fig. 1 (a) The variational energies associated with different stable order parameters for the one-component Bose-Hubbard model. (b) The corresponding phase diagram. 'D' is the dimerized phase with $\langle a^2\rangle = 1/2$ and $\langle a\rangle = 0$; 'SF-D' the superfluid phase with a stable $\langle a\rangle \neq 0$ and unstable $\langle a^2\rangle \neq 0$; 'Mott' is the Mott insulator phase with $\langle a\rangle = \langle a^2\rangle = 0$.

Fig. 2 The phase diagrams for different V/U. 'MS' denotes the molecular superfluid phase with a stable $\langle a_\uparrow a_\downarrow\rangle = \frac{1}{2}$ and other order parameters vanish. 'MS/AS-D' denotes all order parameters non-vanishing but only $\langle a_\uparrow a_\downarrow\rangle$ stable. 'AS/MS-D' does similarly but $\langle a_\sigma\rangle$ stable. (a) The hard-core limit. (b) Finite V/U.


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